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Visible-NIR 'point' spectroscopy in postharvest fruit and vegetable assessment: The science behind three decades of commercial use

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ABSTRACT

The application of visible (Vis; 400–750 nm) and near infrared red (NIR; 750–2500 nm) region spectroscopy to assess fruit and vegetables is reviewed in context of 'point' spectroscopy, as opposed to multi- or hyperspectral imaging. Vis spectroscopy targets colour assessment and pigment analysis, while NIR spectroscopy has been applied to assessment of macro constituents (principally water) in fresh produce in commercial practice, and a wide range of attributes in the scientific literature. This review focusses to key issues relevant to the widespread implementation of Vis-NIR technology in the fruit sector. A background to the concepts and technology involved in the use of Vis-NIR spectroscopy is provided and instrumentation for in-field and in-line applications, which has been available for two and three decades, respectively, is described. A review of scientific effort is made for the period 2015 - February 2020, in terms of the application areas, instrumentation, chemometric methods and validation procedures, and this work is critiqued through comparison to techniques in commercial use, with focus to wavelength region, optical geometry, experimental design, and validation procedures. Recommendations for future research activity in this area are made, e.g., application development with consideration of the distribution of the attribute of interest in the product and the matching of optically sampled and reference method sampled volume; instrumentation comparisons with consideration of repeatability, optimum optical geometry and wavelength range). Recommendations are also made for reporting requirements, viz. description of the application, the reference method, the composition of calibration and test populations, chemometric reporting and benchmarking to a known instrument/method, with the aim of maximising useful conclusions from the extensive work being done around the world.

1. Review objectives

The use of Visible-Near Infrared (Vis-NIR) spectroscopy (Vis-NIRS) to analyze fresh produce (intact fruit or vegetables; referred to as 'fruit' throughout this article) in postharvest applications is a relatively mature topic. The basics of the spectroscopic and chemometric theory is established, and a range of instrumentation dedicated to the post-harvest sector is available. Indeed, in-line Vis-NIR spectroscopic capabilities have been offered by manufacturers of commercial packing lines for nearly three decades, and handheld equipment dedicated to fruit analyses have been available for two decades. However, while technologies such as weight cells and colour cameras are now ubiquitous in pack-lines, adoption of spectroscopic technologies into commercial post-harvest practice to assess chemical properties is still relatively limited. Thus, there is room for confirmation of past work and for further improvements to underpin adoption.

It is also now over a decade since the comprehensive review on Vis-NIRS in postharvest biology by Nicolaï et al. (2007). A review on the same topic was produced by Wang et al. (2015), followed by a similarly scoped reviews by Xie et al. (2016); Kawano (2016) and Cattaneo and Stellari (2019). In the period 2015 to February 2020, a further 18 reviews relevant to the use of Vis-NIR spectroscopy with fruit were published. Some of these reviews were relatively wide in scope, considering applications to food in general (e.g., Aleixandre-Tudó et al., 2019; Cortés et al., 2019; Kumaravelu and Gopal, 2015; Xu et al., 2019), while others review specific commodities (e.g., assessment of thick rind fruit, Arendse et al., 2017; wine grapes, Dambergs et al., 2015; avocado, Magwaza and Tesfay, 2015; olives, Stella et al., 2015) or specific attributes (e.g., detection of insect infestation, Jamshidi, 2019; TSS of a number of fruit types, Li et al., 2016; Magwaza and

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Opara, 2015). Yet other reviews have focused to a consideration of specific techniques applied to fruit assessment, such as data processing (Srivastava and Sadistap, 2018), methods for assessment of light scattering (Torricelli et al., 2015) or to comparison of a range of techniques, including Vis-NIRS, e.g., in assessing fruit ripeness (Li et al., 2018).

The current review is submitted in context of a special edition of the journal of Postharvest Biology and Technology on the use of vibrational spectroscopy in postharvest applications, and focusses to a consideration of 'point' measurements, as opposed to 'area' measurements such as achieved with hyperspectral imaging (for this topic, see the companion review of Lu et al., 2020). The review also focusses the use of the attenuation spectrum of a fruit, i.e., the combination of both absorbance and scattering of photons. For consideration of attempts to separate the two phenomena of absorption and scattering through time or spatially resolved spectroscopy, see the companion review by Lu et al. (2020). The topic of chemometrics is considered only briefly in the current manuscript, given coverage in the companion review by Saeys et al. (2019).

Given the extensive coverage of other reviews, e.g., in tabulating RMSEC and RMSECV achieved for the commodity and attribute assessed in published work, the current review focusses to key issues relevant to the widespread implementation of Vis-NIR technology in the fruit sector, as follows:

Section 2 provides a background to the concepts and technology involved in the use of Vis region spectroscopy in assessment of colour and pigment content, and NIR spectroscopy in assessment of intact fruit attributes with use of chemometrics,.

Section 3 contains a description of commercial instrumentation available for in-line and in-field applications.

Section 4 documents scientific effort published over the period 2015 - February 2020 in terms of application areas, instrumentation, chemometric methods and validation procedures.

Section 5 provides a critique of published work, with suggestions for future work.

Section 6 contains recommendations for documentation of future research activity in this area, to maximise gain in the form of useful conclusions from the extensive work that is being done by many researchers around the world.

2. Background

2.1. Spectroscopy

The Vis and NIR regions of the spectrum span the ranges 400–750 nm and 750–2500 nm, respectively. Of this range, the 750–1100 nm region is referred to as the short wave NIR (SWNIR), or Herschel region, while the 1100–2500 nm region is considered the NIR region proper.

The Lambert-Beer-Bouguer law for dilute, non-scattering solution, as established some two centuries ago, relates absorbance (-log I_t/I_i, where I_t is the intensity of the transmitted signal and I_i is the intensity of the incident signal) to the pathlength, extinction coefficient, and concentration of absorbing analyte. In fresh produce there is, however, a high level of light scattering for light interacting with tissue, increasing the effective pathlength travelled by light and invalidating the eligibility of the Lambert-Beer-Bouguer law. Nonetheless, the attenuation of Vis and NIR radiation from or through fruit has been used for a variety of quantitative applications (e.g., Nicolaï et al., 2007).

Visible region spectroscopy is based on electronic transitions of molecules that result in the absorption of light of matched energy level (i.e., at specific wavelength). The resulting, rather sharp absorption peaks, with typical full width half maximum, FWHM, of approximately 20 nm occur, are hardly affected by temperature (Zude-Sasse et al., 2002). Near infrared spectroscopy (NIRS) involves measure of the absorption of light associated with vibration of molecular bonds. In the assessment of intact fruit, this typically involves absorption associated with the stretching of O—H and C—H bonds (Kawano, 1994; Golic et al., 2003), associated primarily with water and storage reserves (the dominant macroconstituents of fruit). The fundamental absorption bands associated with these features lies in the infrared region (> 2500 nm), with much narrower and higher absorption peaks than associated with the overtones seen in NIR region.

2.2. Vis spectroscopy

The visual colour of a food product is determined by the pigment classes of chlorophylls, carotenes, xanthophylls, anthocyanins and other phenols (De Jager and Roelofs, 1996). Colour is an important quality characteristic for consumer acceptance, either aesthetic or linked to functional attributes and to the developmental stage of the product (Pathare et al., 2013).

Several tristimulus scales based on human perception are used in measurement of colour, e.g., CIELAB, Lch. These color scale values can be correlated to fruit pigment levels. For example, the hue (h) and CIELAB colour parameters a^* and the ratio a^*/b^* were correlated to carotenoids content in apricot fruit (Ruiz et al., 2008) and chlorophyll content in apple (Knee, 1980). Colour space values have also been used in various maturity and ripening indices. For example, Uwadaira et al. (2018) related peach maturity to colour and firmness.

Alternatively, fruit pigments can be assessed based on their spectral

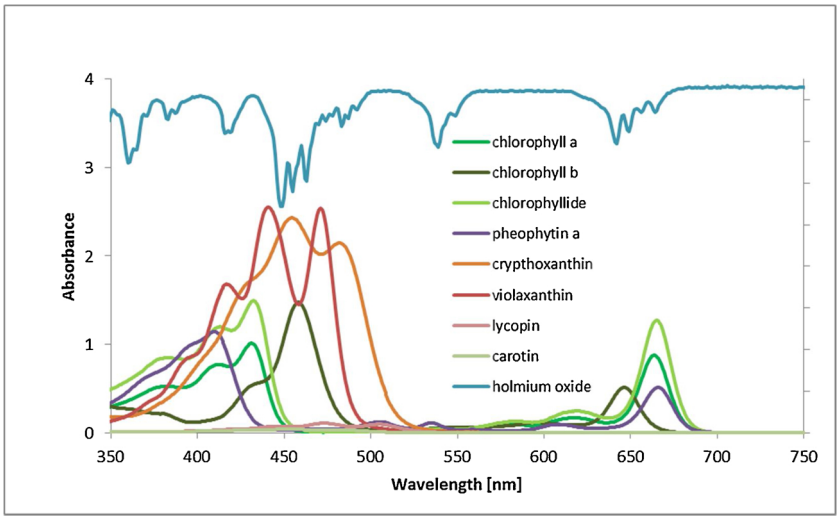

Fig. 1. Absorption spectra of pigments in acetone, and of holmium oxide, used for spectral calibration.

features. Carotenes and xanthophylls absorb with three peak maxima in the wavelength range from 420 to 503 nm (Fig. 1). The common fruit pigment beta-carotene has a yellow to orange-red colour and a strong absorption feature near to 475 nm. The xanthophylls, lutein and violaxanthin, display an absorbance peak at approximately 435 nm, with strong absorption across the 350–500 nm range. Absorbance in the green region around 530–550 nm is caused by an anthocyanin pigment-sugar–protein complex (Merzlyak et al., 2003; Toledo-Martín et al., 2016), e.g., in apples (Iglesias and Alegre, 2009; Iglesias et al., 2012). Chlorophyll absorbance in the blue and red wavelength regions is well described (Kuai et al., 2018). The 680 nm *in-vivo* peak is utilised by various spectral indices and non-destructive analyses implemented in commercial devices for analysing mainly the chlorophyll content of fruit.

Several simple spectral absorption indices have been proposed for assessment of pigments. Many of these indices have been developed in remote sensing applications such as the normalized difference vegetation index (NDVI; Rouse et al., 1973) and the red-edge, and adapted for fruit assessment (Herold et al., 2009) (Table 1). In intact fruit, chlorophyll content has been related to the difference of the intensity of diffuse reflectance measured at 680 and 720 nm for apples (Zude-Sasse et al., 2000), and at 670 and 720 nm for nectarines (DA index, Ziosi et al., 2008). These indices typically involve measurement at a wavelength associated with absorption of the pigment of interest, referenced by measurement at a wavelength that is affected by scattering in the fruit tissue but not affected by pigment absorbance. NDVI is sensitive to low chlorophyll contents such as in ripened fruits, but it and many other indices are saturated at high chlorophyll content (Dash and Curran, 2004). Fruit with high chlorophyll content can be better assessed using the red-edge value (Zude-Sasse et al., 2002; Sims and Gamon, 2003; Dash and Curran, 2004). These approaches are compromised, however, if there are changes in the level of scattering in the fruit, e.g., during ripening (Seifert et al., 2015).

2.3. NIRS

The concept of quantitative determination of analyte level in solid materials using near infrared spectroscopy was established by Karl Norris of the United States Department of Agriculture (USDA) in the 1960s, based on work with low moisture agricultural products (water in grains, Norris and Hart, 1965, later published in Norris and Hart, 1996). USDA work continued into application to high moisture content intact fruit and vegetables, with Birth et al. (1985) publishing on the assessment of the dry matter content (DM) on onions, and the group continuing into assessment of total soluble solids (TSS) of melons (Dull et al., 1989). A research and development program then began in Japan, with the first publication (Kawano et al., 1992) reporting on assessment of TSS on intact peaches.

The absorptivity of the overtones features seen in the near infrared region are lower than those in the infrared. This characteristic is the reason for the use of the NIR wavelength region with intact product, as it allows for effective pathlengths through fruit in the order of millimetres to centimetres rather than micrometres as experienced for wavelengths > 2500 nm. For the same reason, longer effective pathlengths are possible with higher overtone features in the SWNIR region compared to overtones in the NIR region, i.e., with use of the 750 − 1100 nm region over the 1100 − 2500 nm region.

Absorption at 840, 960 and 1440 nm is associated with the first, second and third overtones of O−H stretching, while absorption at 1900 nm associated to a combination O−H feature. The position of the O−H features, however, are affected by the degree of H bonding, and thus by temperature and solute concentration. Absorption near 910, 1100 and 1700 nm is associated with C–H third, second and first overtone features. All absorption features are broad and overlapped, such that interpretation of the raw absorption spectra of fruit is difficult, beyond noting features related to water. The enabler for use of NIRS over infrared spectroscopy was the development of chemometrics, which allowed relevant data to be 'teased out' of the spectra.

3. Instrumentation for Vis-NIR systems

3.1. Visible region devices for colorimetry and pigment spectroscopy

Features to look for the instrumentation for colour measurement include (i) an optical geometry achieving an even, diffuse illumination of the object surface with an integrating sphere, a colour stable illumination source with high end instrumentation utilise Xe flash lamps, while lower cost instrumentation use halogen lamps or light emitting diodes (LEDs) and a full spectrum or tristimulus detector (Table 2). Lamp spectral output can be affected by lamp temperature (Hayes et al., 2014). The most widely used light source standard in colour measurement of food is the illuminant CIE (Commission Internationale de l'Eclairage) D65, which corresponds to the spectral distribution of the midday sun in Western Europe. Instruments using light sources with a

Table 1
Spectral indices relevant to pigment analysis.

Index	Equation	Source
Xanthophyll indices		
Photochemical Reflectance Index (570)	$PRI_{570} = (R_{570} - R_{531})/(R_{570} + R_{531})$	Gamon et al. (1992)
Photochemical Reflectance Index (515)	$PRI_{515} = (R_{515} - R_{531})/(R_{515} + R_{531})$	Hernández-Clemente et al. (2011)
Chlorophyll pool indices		
Red Edge	$ZM = R_{750}/R_{710}$ - 1	Zarco-Tejada et al. (2001); Herold et al. (2009)
Lichtenthaler indices	$Blue/Red = (\rho_{440})/(\rho_{690})$ $Blue/far\ red = (\rho_{440})/(\rho_{740})$	Lichtenthaler et al. (1996)
Vogelmann	$VOG1 = R_{740}/R_{720}$	Vogelmann et al. (1993)
Gitelson and Merzlyak indices	$GM1 = R_{750}/R_{550}$ $GM2 = R_{750}/R_{700}$	Gitelson and Merzlyak (1997)
Pigment Specific Simple Ratio Chlorophyll a	$PSSRa = R_{800}/R_{675}$	Blackburn (1998)
Pigment Specific Simple Ratio Chlorophyll b	$PSSRb = R_{800}/R_{650}$	Blackburn (1998)
Transformed Chlorophyll Absorption in Reflectance Index	$TCARI = 3{\cdot}[(R_{700} - R_{670}) - 0.2{\cdot}(R_{700} - R_{550}){\cdot}(R_{700}/R_{670})]$	Haboudane et al. (2002)
IAD-Index	$IAD = R_{670}$ - R_{720}	Ziosi et al. (2008)
Normalised Difference Vegetation Index (NDVI)	$NDVI = [R_{780} - R_{660}] / [R_{780} + R_{660}]$	Rouse et al. (1972) Zude (2003)
Carotenoids indices		
Structure-Intensive Pigment Index (carotenoid to chlorophyll ratio)	$SIPI = (R_{800} - R_{445})/(R_{800} + R_{680})$	Peñuelas et al. (1995)
Pigment Specific Simple Ratio Carotenoids	$PSSRc = R_{800}/R_{500}$	Blackburn (1998)
Others	R_{520}/R_{500} R_{515}/R_{570} R_{515}/R_{670}	Zarco-Tejada et al. (2012)

Table 2
Examples of handheld chromameters used in assessment of fruit and vegetables.

Instrument	Manufacturer	Light source
CR400[a]	Minolta, Japan	Xe flash
ColourStick[b]	Lincoln University, NZ	broad spectrum (white) LED
Pro Color[c]	Nix, USA	broad spectrum (white) LED
Triad[d]	Agrosta, France	LEDs of 18 wavelengths

[a] https://sensing.konicaminolta.us/products/cr-400-chroma-meter-colorimeter; doa 5/3/20.
[b] https://www.lincolnagritech.co.nz/capabilities/tech-licensing/colourstick-moist-surface-colorimeter; doa 5/3/20.
[c] https://www.agro-technologies.com/ang/produits/spectrophotometer; doa 5/3/20.
[d] https://www.nixsensor.com/compare-nixes; doa 5/3/20.

different spectral output can utilise a conversion factor to achieve a virtual D65 output.

The most widespread electronic, low cost, colour detector is the ubiquitous colour camera. Common CMOS and CCD cameras utilise red, green or blue (RGB) filters centred at 700, 546 and 436 nm, respectively, in a Bayer pattern across individual pixels. These devices were first adopted into electronic packing lines in the late 1970s and are now widely implemented. RGB data can be approximately transferred to the XYZ colour coordinate space and then to other colour spaces such as the CIELAB (Poynton, 1997). Alternatively, XYZ values can be calculated from a 400–700 nm spectrum, typically using data at 5 nm steps, but CIE (1986) also provides colour tables at 1 nm resolution. In practice, e.g., for sorting purposes on packlines, RGB values are used directly.

Achieving a more direct match to a colour space, several 'tristimulus' colorimeters capture light in wavelength ranges matched to the colour coordinate system of interest with the use of filtered photodetectors, e.g., the 'industry standard' Minolta CR400 (www.minolta.com) (Table 2). The expense of such specialty filters, however, can add greatly to the overall cost of an instrument.

The tristimulus devices are also not appropriate for complex colour analysis such as metamerism and colorant strength. The standardised assessment of colour can be achieved using a spectrophotometer based on Si photodiode or CMOS technology, which may measure beyond the visible range into SWNIRS (e.g., the ST from Ocean Optics, https://www.oceaninsight.com/products/spectrometers/microspectrometer/sts-series; doa 5/3/20), given appropriate lighting.

Low cost LED based instrumentation for assessment of 'colour' is becoming available. For example, the Colour Stick employs a diffuse white LED source and four photodetectors (RGB filters and a clear channel), with output using various colour spaces (pers. comm. Paul Riding, Colour Stick; Table 3). The Agrosta fruit spectrophotometer uses LEDs of 18 peak wavelengths that sequentially illuminate the fruit, with use of a single detector (https://www.agro-technology.co.uk, doi 5/3/2020), providing 'colour' defined in terms of the 18 remittance values rather than in terms of a colour space such as CIELAB.

Several LED based instruments have also been released that target assessment of specific pigment in fruit (Table 3). The DA meter, Kiwi meter and Cherry meter measure at two or three wavelengths aimed at chlorophyll or red pigment detection. The MultiPlex operates using several wavelengths, with several indices to address a range of pigments. While the Multiplex employs a diffuse reflection optical geometry, the Turoni devices and the FIORAMA probe operate using a partial transmission geometry and the IDD4 utilises a full transmission geometry in a packline application, for assessment of internal defects such as internal browning (Table 4).

3.2. SWNIRS in-line equipment

In-line applications are characterised by constraints related to speed of assessment, appropriate to packline conveyor speed, to the geometry of the conveyor belt and to operating conditions (e.g., vibration). On a positive note, ambient light conditions can be reasonably controlled using a housing over the conveyor system, in contrast to spectrometers intended for in-orchard use. The first commercial use of NIRS technology was in Japan, beginning in the late 1980s/early 1990s, with use for in-line sorting of fruit on attributes such as Total Soluble Solids (TSS) (Walsh, 2005). The first providers of in-line NIRS equipment included Mitsui Metals and Mining, Sumitomo, Fantec and Emitec (all of Japan). The early systems utilized reflectance optics, but this geometry was soon replaced by partial or full transmittance optics, presumably due to model robustness issues associated with a reflectance geometry. All systems utilized halogen lamps, with the notable exception of the Sumitomo system, which utilized diode lasers. This product was discontinued, presumably due to the added cost and to issues associated with stability of laser output intensity. Technology adoption continued in the new century (early 2000s), with release of in-line equipment by the global grading equipment manufacturers, Colour Vision Systems (Australia, now part of MAF RODA, France) and Compac (now part of Tomra, Norway), and later, Greefa (Holland), Multiscan Technologies (Spain), Aweta (Holland), Sacmi and Unitec (Italy).

Current 'state of art' commercial systems achieve assessment of fruit travelling at a belt speed of 1 $m.s^{-1}$ with simultaneous operation of multiple lanes, with sorting of up to 10 fruit per second (depending on fruit size). Current systems employ a SWNIR spectrophotometer, i.e., operate to approx. 1050 nm, in partial or full transmission geometry. Issues relevant to in-line application include: (i) the influence of the movement of the samples during the measurement interval, e.g., a 20 ms integration time involves movement of the fruit by 20 mm during assessment at a 1 $m.s^{-1}$ belt speed; (ii) use of an optical geometry that minimizes the impact of changing fruit size and shape (including minimizing specular reflectance received by the detector); (iii) measurement of a representative portion of the fruit, given natural internal distribution of the constituents; and (iv) robust chemometric models

Table 3
Dedicated multi wavelength meters used in assessment of fruit and vegetables.

Instrument	Format	LED peak wavelengths (nm)	Optical geometry	Application
DA meter[a]	handheld	670, 720	remittance	chlorophyll
Kiwi meter[a]	handheld	560, 640, 750	remittance	red pigments
Cherry meter[a]	handheld	560, 640, 750	remittance	red pigments
MultiPlex330[b]	handheld	435, 685, 735	diffuse reflectance	pigments
SoftRipe[c]	handheld	660, 720	diffuse reflectance	chlorophyll
FIORAMA[d]	handheld	535, 570, 685, 720, 950	remittance	chlorophyll, red pigments
IDD4[e]	in-line	4 wavelengths	transmittance	internal defects

[a] T.R. Turoni Srl., Forlì, Italy; https://www.trturoni.com/en/fruit-veg-ripeness-quality-control/da-meter; doa 5/3/20.
[b] Force-A, Paris, France; https://www.force-a.com/fr/produits/multiplex ; doa 5/3/20.
[c] Frigotec GMBH, Landsberg, Germany; https://softripe.com/discover/ripening-technology/home; doa 5/3/20.
[d] CP, Potsdam-Golm, Germany; http://cp-info.de/Our-Products; doa 5/3/20.
[e] MAF, Montabaun, France; https://www.maf-roda.com/en/page/electronic-sorting.php; doa 5/3/20.

Table 4
Commercially available portable Vis-NIR spectrophotometers.

Technology	Manufacturer, model	Wavelength range (nm)
Dedicated fruit spectrometers		
grating and CMOS array based spectrometer, halogen lamp, partial transmission	SunForest (Korea)	790 – 950
	Felix Instruments, F751 (USA) (www.felixinstruments.com)	330 – 1100
grating and Si diode array based spectrometer, halogen lamp, partial transmission	Sacmi, (Italy) (http://www.sacmi.com)	650 – 1050
	Felix Instruments, F751	330 – 1100
	K-BA-100R1, Kubota (Japan) (jnouki.kubota.co.jp/product/kanren/fruit_selector/)	500 – 1000
Si detector, 20 LEDs of 6 wavelengths, partial transmission	Atago, Hikari (Japan) (atago.net/product/)	na
Generic miniature spectrometers		
linear variable filter, halogen lamp, reflection	Viavi, MicroNIR (USA) (www.viavisolutions.com/en-us/osp/products/micronir-spectrometers)	900 – 1700
Digital light projector (DLP), reflection	SG1 (Taiwan) (www.ti.com/tool/TIDA-00,155)	900 – 1700
Fabry-Perot filter inferometer grid and image sensor with 12 receptors, diffuser/plate with holes of different aperture sizes/lens, broad region LED, reflection	SCiO (Israel) (www.consumerphysics.com/scio-for-consumers/)	
plasmonic filter - a metal film perforated with subwavelength 32 × 32 hole arrays directly on the light sensor array IC, reflection	NanoLambda (Daejeon, Korea); (www.nanolambda.myshopify.com/)	390 – 760
Fourier Transform using Mach-Zehnder interferometers, reflection	(www.fringoe.com/fringoe-spectrometer)	
MEMS, reflection	Thermo, Phazir 2400. (Wilmington, MA, USA) (www.thermofisher.com/order/catalog/product/MICROPHAZIR)	1600 – 2400
MEMS-FTNIR Michelson interferometer, reflection	Si-Ware (Cairo, Egypt) (www.neospectra.com/)	1350 – 2500

(Cortés et al., 2019).

Due to commercial sensitivities, performance benchmarking of the commercially available equipment is not available in the scientific literature, with (to the authors knowledge) the exception of Walsh et al. (2020). Attempts have been made to emulate issues relevant in-line systems, e.g., Ignat et al. (2014) compared performance of PLSR models on apple attributes for static and moving fruit using two different spectrometers. Unfortunately, attempts to emulate in-line systems in scientific reports are often misguided in use of design features not used in commercial instrumentation, e.g., reflectance optics or wavelength ranges beyond 1050 nm (e.g., Ignat et al., 2014; Salguero-Chaparro and Peña-Rodríguez, 2014).

However, although a range of instrument manufacturers have supplied the fruit and vegetables market for some decades, commercial adoption has been relatively modest relative to adoption of technologies such as machine vision and load (weight) cells. The resistance to uptake can be attributed to three factors: (i) achievable accuracy and precision, (ii) operational complexity and (ii) value created. Unlike the direct measurement of an attribute such as weight on a packline, visible-NIRS measurements are indirect, and the strength of the indirect relationship is stronger for some attributes in some applications than others. This uncertainty requires a higher level of management effort. Operational complexity relates to the need for regular calibration (model updating) of the equipment, which if not undertaken will compromise the reliability of operation (e.g., Walsh et al., 2020). An example of value created is seen in the Japanese gift fruit market which rewards premium internal quality. This 'pull factor' underpinned early technology uptake in Japan with exceptionally high prices. However, improved eating quality (e.g., higher TSS) is not associated with significant premium pricing in many markets. In western countries, a greater market pull exists for sorting for removal of internal defects for which there is a strong penalty (e.g., consignment rejection if incidence of apple internal browning exceeds 2%). Uptake of NIR sorting has thus favored defect sorting applications in western markets, despite the level of uncertainty in assessment (e.g., Khatiwadi et al., 2016).

3.3. SWNIR devices for handheld use

These are a number of models of dedicated handheld 'fruit spectrometers' on the market which provide for calculation and display of the predicted level of an attribute on the device and are physically designed for use with fruit (Table 5). A primary difference for a field spectrometer compared to a unit designed for indoor use is tolerance of variation in ambient light levels (sunlight) and temperature. A range of generic, i.e., not specific to fruit, miniature spectrometers have also been released, with promotional material often providing examples of fruit assessment (Table 4). Luggable or handheld equipment purpose built for fruit assessment in field became commercially available in the early 2000s, with instruments released by Fantec (Japan), CP (Germany), Sacmi (Italy), Integrated Spectronics (Australia), Kubota (Japan) and later, Felix Instruments (USA). While Fantec (NIRGun), Integrated Spectronics (Nirvana) and CP (Pigment Analyzer) have exited this field, recent releases targeting the handheld market include the GWon (Korea), SunForest (South Korea), Atago Hikari (Japan) and FHK (Japan) (Table 4).

The 'fruit spectrophotometers' are most commonly based on a tungsten halogen light source, a grating and Si photodiode or CMOS linear array detector, operating within the range 350–1100 nm and a partial transmission (interactance) geometry. Referencing with every sample can be used to accommodate variation in ambient light level.

A range of alternative detector technologies (see review by Yan and Siesler, 2018; also Table 4) have been released and others are in development. These technologies have been deployed within generic use spectrometers, but they have yet to be utilised in systems dedicated to fruit assessment, with appropriate optical geometry, wavelength range and graphical user interface. Such adaption can be expected over the next decade.

For example, the Atago and SCiO devices employ LEDs as short wave near infrared region (SWNIR) light sources, using less power and avoiding the need for heat dissipation systems inherent in the use of a halogen lamp, the classical light source for NIRS systems. The cost of doped InGaAs based detectors has decreased, enabling use of this technology for applications requiring a longer NIR wavelength region (e.g., 800 – 2400 nm). Light dispersion technologies such as a linear variable filter (as used in the MicroNIR, Viavi) can allow for a more compact instrument design than achieved with use of a grating. Bao and Bawendi (2015) produced a quantum dot spectrometer chip by printing quantum dot inks on the surface of a detector array, allowing multiple spectral bands to be encoded and detected simultaneously with one filter and one detector. This type of spectrometer is small enough for use in a mobile phone. FTNIR, which uses an interferometer and a single detector, provides a different approach to wavelength dispersion. This technology holds advantages over other dispersive technologies in optical resolution achieved and is promoted as providing ease of model

Table 5
Example of publication metadata records.

References	Commodity	Attribute assessed	Wavelength range (nm)	Optical geometry	Statistical method	Test set
Rady et al. (2018)	Carrots	colour, firmness, moisture content TSS, Vitamin C, ß-carotene	400 – 1000 900 – 1700	reflection	PLSR	population of calibration set
Xiao et al. (2018)	Grapes	maturity (colour, TSS, phenolic compounds)	400 – 1100 900 – 2500	reflection	LS-SVM, PLS, CARS, SVM-DA	population of calibration set
Huang et al. (2018a)	Tomato	maturity (firmness)	400 – 1100 900 – 1683	partial transmission	PLSR	population of calibration set
Tilahun et al. (2018)	Tomato	lycopene, ß-carotene	500 – 1100	full transmission	PLS	population of calibration set

transfer between instruments. Micro-Electro-Mechanical Systems (MEMS) have been used in micromirror arrays (so called Digital Light Processors, DLP) to create compact dispersive elements that can then be coupled to other optics and detector elements to create miniature micro-opto-electro-mechanical systems (MOEMS) based spectrometers, as used in the SCiO, SG1 and Phazir instruments.

4. Scientific effort (2015–2020)

While spectrophotometric assessment of fruit has been in commercial use for over thirty years, scientific community activity, as indexed by publication output recorded by Scopus (http://www.scopus.com), has increased dramatically in the last 15 years (with 310, 804 and 863 publications in the previous 5, 10, and 30 years, respectively, given keyword search as detailed in Fig. 2). This increase in output is underpinned by the availability of instrumentation, with advances in relevant technology, including miniaturisation, detector types, low power use light emitting diodes, computing speed and chemometric data analyses, wireless communication and cloud computing are underpinning new generations of instruments at a budget that is affordable for producers, consultant services and other post-harvest stakeholders. Over the last decade, output of around 80 publications per annum has occurred.

Journal publications from 2015-Feb 2020 (n = 316) were categorized on the commodity and attribute assessed, the wavelength range and optical geometry of the instrumentation used, the chemometric modelling technique and the validation procedure employed (Table 5;

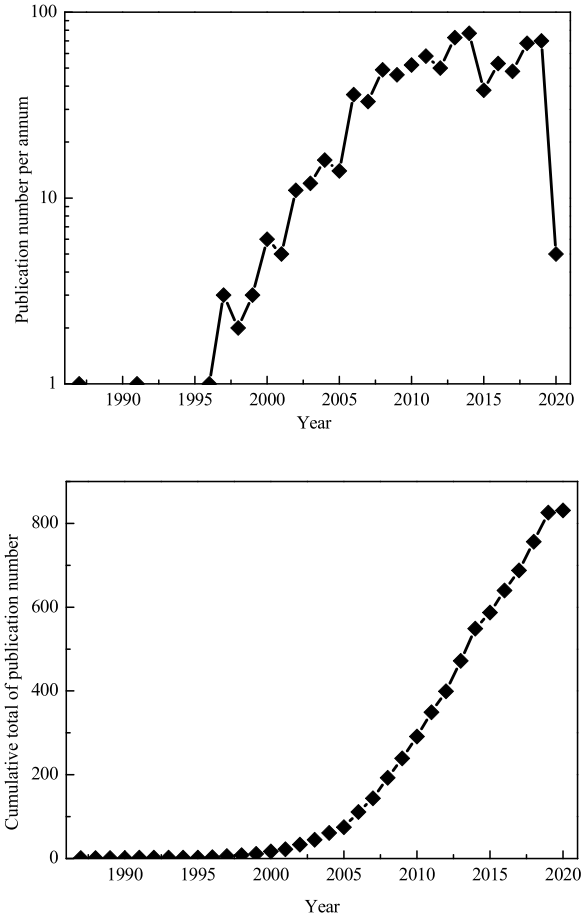

Fig. 2. Scopus record as of 02/2020 on documents using the keywords “visible” or “near infrared” or “spectroscopy” and “fruit”, with exclusion of “metal nanoparticles” and “plant extracts”. Top panel: publication number per annum on a log scale. Bottom panel: cumulative total of publication number.

Table 6
Publications on visible or near infrared spectroscopy over the period Jan 2015 - Feb 2020, segregated by topic (in terms of number and percentage). Note that a given publication can be scored in several categories (e.g., if it involved several fruit types).

Commodity	#	%	Attribute	#	%
Citrus	33	12	TSS	135	32
Pome	75	26	Dry matter	32	7
Stone	50	18	Acidity	62	14
Tomato	25	9	Firmness	42	10
Other	102	36	Color, pigment	42	10
			Internal defect	30	7
			Species, variety, origin	27	6
			Maturity, ripeness	24	6
			Other	76	18
Wavelength range (nm)	**#**	**%**	**Statistical method**	**#**	**%**
< 1050	108	43	Partial least-square (PLS)	198	45
< 1700	33	13	Support vector machine (SVM)	41	9
< 2500	112	44	Discriminant analysis (DA)	76	17
Full range	147	56	Other	127	29
Variable selection	116	44			
			Test set	**#**	**%**
Optical geometry	**#**	**%**	Cross validation only	185	66
Reflection	210	75	Dependent test pop	62	22
Partial Transmission	54	19	Independent test pop	32	11
Full Transmission	16	6			
			Cross validation	**#**	**%**
			Leave one out	134	68
			Group based	62	32

full metadata table available on request from authors) with the number of publications per category presented in Table 6. Papers using multi- or hyperspectral imaging only (n = 35 for this period and keyword search) were excluded. Most papers originated from China (45 %), followed by United States (8 %), Spain (8 %), Italy (6 %), and Japan (5 %).

Over the period 2015 to Feb 2020, Vis-NIR spectroscopy was reported in measurement of a range of post-harvest attributes of fruit including moisture content, pigmentation (anthocyanins, carotenoids, chlorophylls), storage reserve level (soluble sugar, starch or oil), organic acid levels, various internal defects (internal browning, glassiness, stone cracking, bruising, bitter pit, internal rots), maturity indices, and claims were made for measurement of firmness and more indirect analyses.

Pome fruit, particularly apple, received the most attention in these publications, followed by stone fruit and citrus, with TSS being the most investigated attribute (29 % of reports, Table 6). Acidity and firmness featured in 22 % of all 2018 publications. The majority of publications reported use of a wavelength region above 1050 nm (61 %) and a reflection geometry (75 %). PLS was the dominant multivariate regression method in use (45 % of publications), with only 11 % of reports employing an independent test population. Where cross validation was used, (33 %) of reports used the leave-one-out procedure.

A proportion of the published papers are 'derivative' in that they demonstrate application of an existing technique to a different fruit commodity, e.g., a 'known' wavelength selection or multivariate analysis technique. While incremental improvements and documentation of Vis-NIRS applications to a given commodity-attribute are useful to support adoption of the technology, there are additional requirements to provide a useful addition to scientific literature. The following sections attempt to document such requirements, and also highlight differences between Vis-NIRS technology used in commercial postharvest practice and the weight of scientific studies (Table 6). These differences may reflect cost and ease of implementation pressures on commercial practice, at a compromise to performance, or alternatively the differences may reflect the instrumentation and resourcing available to researchers.

5. Visible-NIR spectroscopy and colour assessment

5.1. Definitions

Nomenclature for the geometries of light source, sample and detector has been described in previous reviews (e.g., Chen, 1978; Nicolaï et al., 2007; Herold et al., 2009), but as the terminology is often confused in postharvest literature the terms are briefly repeated here (Fig. 1). By IUPAC definitions, the terms 'reflectance', 'interactance' and 'transmittance' refer to the quantity of light received from a 'reflection', 'interaction' and 'transmission' optical geometry. The term 'attenuance' (formerly termed extinction) is analogous to absorbance but encompasses scattering and luminescence (Cohen et al., 2008; Verhoeven, 1996). 'Apparent absorbance' is an equivalent term to attenuance. The term 'remittance' is also sometimes used, referring to the quantity of light that is received by the detector, being used in context of partial transmission geometry. The terms reflection, transmission, interaction and remission refer to the geometry involved (Fig. 3).

In a reflection geometry, the detector views an illuminated part of the fruit, receiving both specular and diffusely reflected light ('reflectance'). Specular reflections carry no information on the internal attributes of the sample. The intensity of the 'useless' specular

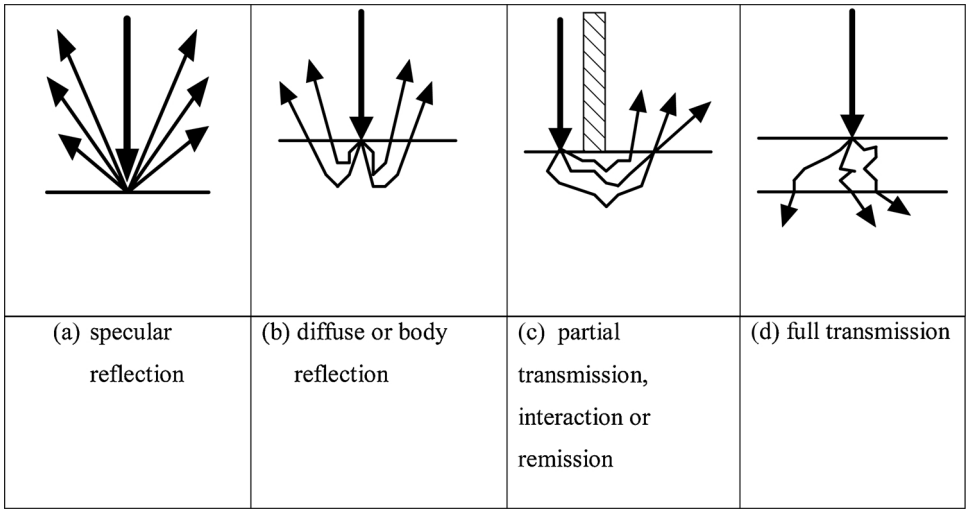

Fig. 3. Representation of potential pathways of light interacting with a sample, depicted with a single incident ray.

reflections seen by the detector can exceed the detected diffusely reflected light in a poorly designed system. A 45° angle between detected rays, collimated illuminating rays and a planar surface will minimise the proportion of specular rays received by the detector. A fundamental limitation to application of a reflectance geometry, however, is that most of the detected diffusely scattered light will have emanated from the superficial layers of the fruit, rather than from the mesocarp which is generally of interest in assessment of fruit internal quality (see further discussion at 4.4).

In transmission geometry, lamp, sample and detector are arranged such that light must pass through the sample to the detector, with no light passing directly from lamp to detector. Such arrangements can involve 180° geometry of lamp-sample-detector ('full transmission' geometry) or lesser angles ('interactance', 'remission' or 'partial transmission'). The 'shadow probe' configuration (Greensill and Walsh, 2001) is a specific partial-transmission geometry that is of use in non-contact assessment of a sample, as required for moving fruit on a packline. In this geometry, an optical probe is placed in front of a collimated light source, creating a shadow on the fruit which is viewed by the probe, with detected signal relatively independent of detector to sample distance. A limitation to use of a 180° transmission geometry with many fruit types is fruit optical density and tissue inhomogeneity. The former issue requires use of strong illumination sources and/or sensitive detectors, while the latter results in a mis-match of the optically sampled volume (i.e., fruit skin, flesh and core) to the attribute of interest (e.g., flesh TSS).

Point spectroscopy provides the sum signals of attenuation, i.e., of absorption and scattering. The scattering properties of a tissue influence the effective path of photons, and thus the effective depth of penetration of light into that tissue and the effective pathlength between the light source and the detector (Cubeddu et al., 2001). However, the amount of scattering differs between fruit types (Cubeddu et al., 2001; Lu et al., 2019) and may change during fruit development (Qin and Lu, 2008; Nicolaï et al., 2008; Zerbini et al., 2015; Seifert et al., 2015). If scattering properties of a fruit change, as shown for European plum during ripening (Seifert et al., 2015), apparent absorption will be changed, upsetting any relationship between apparent absorbance and an attribute of interest. A number of studies have attempted to correct for the perturbations related to scattering, through the use of indices or chemometric data pre-treatments when entire spectra are available (e.g., Sun et al., 2020a, 2020b). Attempts to estimate scattering coefficients and the correct attenuation data to achieve 'true' absorption data, however, have rarely resulted in better correlations between Vis-NIR spectra and attribute levels (e.g., Nguyen Do Trong et al., 2014).

The 'depth of penetration' of light into a sample is defined (Verhoeven, 1996) as the inverse of the decadic absorption coefficient, i.e., the depth at which radiant power is decreased to one tenth of its incident value. Characterisation of this attribute for a given application is useful, towards understanding of the volume of the sample that is optically sampled. Peirs et al. (2003) describe a useful empirical technique based on slices of fruit to assess this characteristic. Methods to easily model light distribution through tissue for a given optical geometry and sample would also be helpful, aiding understanding of the 'optical sample' achieved with a given optical geometry and sample (fruit) type.

5.2. Optical geometry applied in recent years

The choice of optical geometry for a given postharvest application should be informed by a consideration of fruit structure in context of the optical geometry of the spectrophotometric system. The overwhelming majority (75 %) of studies published since 2015 that use Vis-NIRS to assess internal attributes of fruit have employed a reflection geometry, yet such a geometry is not used in any commercial spectrophotometer targeted to fruit application (Section 3). This may be a result of available instrumentation in research laboratories, with a reflection geometry dominating instrumentation used in food applications (Aleixandre-Tudó et al., 2019). Most food applications involve a homogenized material for which a surface (reflection) assessment can be representative of the whole sample. Future reports on application development using Vis-NIRS for fruit attribute assessment should therefore include justification of the optical geometry employed.

Vis-NIR spectroscopy of intact fruit requires the passage of light through fruit 'skin' (typically exocarp and non-edible mesocarp), edible mesocarp and back out through the skin. Spectra acquired using a reflection geometry will carry primarily surface information about the sample in terms of both specular and diffusely reflected light. Variation in fruit shape and surface features will impact the level of specular reflection, affecting apparent absorption values. As specular light is identical to the incident light, its contribution to the apparent absorption spectra can be 'physically' removed by use of polarizing filters, or mathematically removed using pre-treatments such as a derivative. The latter process, however, does not allow for improvement of the signal to noise ratio of the diffuse reflection component.

The diffuse reflected radiation will emanate in majority from within 5 mm depth of apple fruit (e.g., Lammertyn et al., 2000; Peirs et al., 2003) and from less depth for fruit with a denser (higher scattering coefficient) skin such as avocado. Assessment of internal attributes using a reflection geometry therefore requires a correlation between the internal attribute and spectra of external layers of the fruit (as assessed by the reflection geometry).

The use of transmission or interaction geometries seems more appropriate for acquisition of useful spectral information from greater depths of the fruit, relative to use of reflectance geometries. This was demonstrated by Schaare and Fraser (2000) who ranked an interaction, 180° (light-sample-detector) transmission and reflection geometry in the order of highest to lowest performance for assessment of TSS of intact kiwifruit. The reflection result was compromised by the level of specular reflection and superficial layer diffuse reflection, and the transmission result was compromised by either the low detected signal (poor signal to noise ratio) or the impact of seeds and other central zone tissue on the measurement. It is also expected that models based on a reflectance geometry will be less robust in prediction of independent populations than those based on transmittance geometries, being sensitive to change in surface reflectance.

It is thus no surprise that the NIRS technique is suited to thin skinned fruit with homogenous mesocarp (e.g., stone fruit, pome fruit, mango) and that the optical geometry employed must be matched to the fruit type and the signal level (Walsh et al., 2004).

Assessment of internal defects usually requires a pass/fail (discriminant) decision. However, the defect may not be uniformly distributed within the fruit. A reflection geometry involves assessment of one area of the fruit. With a full 180° light-sample-detector geometry, light is scattered within the fruit, including a level of reflection from the internal surface of the skin, and thus this geometry effectively involves assessment of a greater proportion of the fruit volume (Fraser et al., 2003). This geometry may therefore provide a better result than other geometries, as reported in assessment of internal browning of apple (Khatiwada et al., 2016) and pear (Sun et al., 2016), and internal rot in citrus (Lorente et al., 2015).

Several approaches have been attempted to remove the influence of the skin from fruit spectra, including approaches involving combined reflection and transmission measurements (Krivoshiev et al., 2000) and subtraction of a mean skin spectrum. Attempts to estimate the true absorption coefficients, separated from scattering coefficients, for correlation to the attribute of interest are logical (e.g., Lu et al., 2019), but have not resulted in practically relevant solutions to date. Further work is appropriate in this area.

5.3. Optical and reference sampled volume

While 'point' refers to assessment of a point on the fruit surface, the

detected light received carries information on some proportion of the fruit. The volume of the fruit that is 'optically' sampled is dictated by the optical geometry employed, the scattering of light within the sample, and sample movement (e.g., for fruit moving past a detector on a pack line). For example, with in-line assessment, the movement of fruit past the spectrometer results in assessment of a larger volume of tissue than a stationary assessment.

The application of NIRS to assessment of an attribute for a given fruit commodity should therefore also be accompanied by a description of the distribution of the attribute of interest and the likely path of light for the chosen optical geometry, together with a justification for the chosen geometry and the volume of tissue physically sampled for analysis using the reference method. This requirement was recognized early in the application of NIRS to fruit assessment (Peiris et al., 1999), but is lacking in many contemporary reports. An example is provided in the report of Jantra et al. (2017), who note variation of the attribute of interest (TSS and DM) within onion in context of the optical geometry used. Another example is provided by Long and Walsh (2006) for a Vis-NIRS application on intact melon, in which the optically sampled volume was of the outer (inedible) mesocarp only for the instrumentation employed, while the attribute of interest was on inner mescocarp TSS. Thus NIR-TSS predictions were heavily influenced by the correlation of inner and outer mesocarp TSS, which varied with fruit development.

If the optically sampled volume does not represent the whole fruit, consideration should be given to the intent of a sampling regime. For example, the blush (sun) side of fruit typically has higher TSS and chlorophyll than the non-blush (shade) side (Kuckenberg et al., 2008). Thus, a program to assess average TSS of a consignment of fruit should consider either measurement of only blush or non-blush side, or of both. Alternatively, an optical geometry could be employed that assesses the whole fruit, e.g., multiple point measurements. For example, Trong et al. (2013) employed spatially resolved spectroscopy, with several measurements made of each fruit, achieving a TSS prediction $R^2 > 0.83$ against refractometer TSS assessed of juice of the whole fruit.

5.4. Spectrophotometer characterisation

The results of a spectrophotometric based study will be heavily influenced by the instrumentation used, as instrumentation is not 'equal' in performance. Scientific reports should therefore provide a justification for the choice of the spectrophotometric system employed, in context of the application. Reports should also provide detail on instrumentation characters to better allow comparison between studies. For example, Huang et al. (2017) provided relevant descriptions in comparison of CCD detectors for assessment of anthocyanins in mulberry fruit.

Reportable characters include the optical geometry employed, wavelength range, optical resolution, dynamic range and repeatability. Geometry and wavelength range are commonly reported. Optical resolution can be assessed as FWHM of HgAr lamp line spectra. This characteristic is a function of the optical bench of the spectrometer. Note that it is not the same as the pixel resolution or read out wavelength step. Dynamic range provides an index of the intensity resolution of the spectrometer, often quoted as maximum signal divided by baseline (dark) noise measured at the shorted exposure time of the system.

Repeatability can be indexed as the SD of absorbance of repeated measures (e.g., n = 20) of a reference tile. Repeatability will be impacted by the signal and signal to noise level of the detector, variations in lamp intensity and changes in the level of stray light.

'Stray light' in a spectrometer represents 'unwanted' reflections that occur within the the optical bench of the spectrometer, i.e., reflections from photons not following the intended path from input light source to detector. Together with detector noise, stray light sets a limit to the sensitivity of a system. For example, if 1 % of light received by the detector is stray light, the system can not assess absorbance values of greater than 2 units (i.e., the system can not distinguish a signal at 1% of a reference value when there is background noise from stray light at 1% of total light).

Continuing instrumentation advances promise lower cost and easier use of Vis-NIRS within postharvest applications. Appropriately designed comparative studies to existing documented equipment (e.g., Kaur et al., 2017; Subedi and Walsh, 2020) will provide value to the postharvest community, supporting adoption of appropriate technologies. Such instrument benchmarking exercises should describe performance of the instrument with variation in instrument temperature, ambient light levels or vibration and the impact of instrument ageing (e.g., Acharya et al., 2016). Consistency of performance across different units of the same make and model of instrument should also be demonstrated, as demonstrated in the comparative study undertaken by Kaur et al. (2017).

With an increasing array of instrumentation available, it becomes more important to document the characters of the instrumentation used. This is a weak point for most published studies, in terms of both the description of the instrumentation characters and the justification for the choice of instrumentation. In summary, instruments are not 'equal' in performance, so the interpretation of the comparison of instruments differing in wavelength range or optical geometry must be tempered by consideration of these characteristics.

Documentation is also required of the requirements (e.g., wavelength resolution, repeatability) required for a particular application. For example, a requirement for an optical resolution at least 10 nm and a repeatability (SD of repeated reference spectra) of at least 10 mAbs was documented for the application of NIRS assessment of fruit TSS (Greensill and Walsh, 2000). Higher optical resolution and detector pixel resolution can be useful for calibration transfer between instruments. Thus, it is claimed that calibration transfer between FTNIR instruments is more successful than between diode array instruments, as FTNIR provides higher wavelength accuracy optical resolution (Andersen et al., 2013).

5.5. Applications of vis spectroscopy

There has many reports of non-destructive pigment analysis in horticultural applications, from macroscopic studies on plastid development (e.g. Sadali et al., 2019) to interaction with ethylene (Dar et al., 2018), both relevant for determining the optimum harvest date and shelf life prediction. These studies of the assessment of fruit pigmentation have been based on association to colour space values, to absorption indices of a few (usually two) indices and to multispectral analyses.

Visible region assessment of the chlorophyll content of fruits has been reported by many authors over many decades (Olsen et al., 1969; Merzlyak et al., 1999; Zude-Sasse et al., 2002; Zude, 2003; Ziosi et al., 2008), including on tree assessments (Herold et al., 2009). Various two-wavelength indices have been used for chlorophyll content of fruit (e.g., Table 3; Kuckenberg et al., 2008). More recently, fruit chlorophyll analysis has become intensively studied in proximal sensing aimed at phenotyping (Li et al., 2018), which is enabled on single fruit due to recent developments in 3D point cloud analyses with spectral intensity data (Tripodi et al., 2018; Tsoulias et al., 2020).

Red pigments are particularly interesting for both the visual appearance and the health benefits of fruit (e.g., Ilahy et al., 2019). For example, Acharya et al. (2017) and Tilahun et al. (2018) reported prediction of lycopene and ß-carotene content of tomato fruit using PLS models based on Vis-NIR spectra to be slightly superior to predictions based on CIE a*/b* colour coordinates.

Other spectral indices target have been developed for assessment of fruit maturity, based on pigment levels and colour. For example, the citrus colour index (CCI) is based on Hunter Lab values for fruit skin (Jiménez-Cuesta et al., 1981) (eqn. 1).

$$CCI = \frac{100 \cdot a}{L \cdot b} \quad (1)$$

Zude-Sasse et al. (2000) proposed a simple maturity index (MI) for apple (eqn. 2), based on firmness (f), reflectance at 720 (R_{720}) and 680 nm (R_{680}) and the starch index (SI),

$$MI = \frac{f(R_{720} - R_{680})}{SI} \quad (2)$$

The use of visible region spectroscopy for intact fruit pigment analysis is made difficult by the overlapped spectral features associated with the various pigments (Fig. 1) and by scattering (Taroni et al., 2003). Wellburn (1994) developed a simple algorithm to account for the over-lapping absorption spectra of extracted pigments in lipophilic solution. This approach was extended to measurement of chlorophylls and carotenoids in fruit extracts, enabling analysis of chlorophyll *a* and *b*, and carotenoids (Nagata et al., 2007) and chlorophyll *a* and *b*, pheophytin a and carotenoids (Pflanz and Zude, 2008) in one extraction step. This approach has been applied to intact fruit with much lower success (Pflanz and Zude, 2008), but may become applicable once the absorption spectrum is distinguished from scattering spectrum with time or spatially resolved spectroscopy.

Another measurement issue is associated with the variation in pigment spectra that can *in-vivo*. For example, binding of chlorophyll by NADPH affects the electron excitation energy, and, therefore, the wavelength at which the chlorophyll molecule absorbs. During fruit development, the red region peak maximum of chlorophyll absorption can change by 2.3 nm (Seifert et al., 2014). Repots claiming use of a spectral assessment should therefore demonstrate robustness of the method across the range of conditions expected in application.

In general, a RMSEP of 7% and 6% (fresh weight basis) for total chlorophylls and anthocyanins, respectively, can be expected using Vis spectroscopy (Zude-Sasse et al., 2011), considering that the absorbance features of anthocyanins do not overlap with that of the carotenoids.

5.6. NIR assessable attributes

Dry matter and TSS: There is consensus in the literature (from the 316 papers reviewed, Table 7) that Vis-NIRS can be used to assess the macro-constituents of dry matter content and TSS in intact thin-skinned fruit to a RMSEP of less than 1% for both these constituents, and that temperature can be assessed to a RMSEP of approximately 1 °C. Indeed, the use of Vis-NIRS in assessment of fruit dry matter content and TSS of thin skinned fruit is established in commercial practice.

Dry matter content is used as an index of: (i) storage reserves, be that the sum of starch and soluble sugar content, e.g., in pre-harvest apple or mango, or of oil content, e.g., in avocado or olive fruit; and (ii) future soluble sugar content in climacteric fruit storing starch, i.e., after ripening with conversion of starch to sugars, as seen in ripened apple or mango fruit. Thus, dry matter content of fruit at harvest is related to future eating quality.

Some supply chains now set specifications on fruit dry matter content at harvest, with assessment undertaken using NIRS (e.g., Australian Mango Industry Association, 2019). Accumulation of fruit dry matter is also useful in gauging fruit harvest maturity, with the target dry matter level adjusted by growing condition, e.g., in durian (Timkhum and Terdwongworakul, 2012) and mango (Subedi et al., 2007; Anderson et al., 2017).

The relationship between the attributes of dry matter content and TSS is complicated by the presence of insoluble components. The NIRS measurement of fruit TSS involves spectra collected on intact fruit and TSS commonly based on measurement of the refractive index of extracted juice, i.e., ignoring the insoluble components of the fruit. Consider that a fruit of 1 kg weight with 15 % dry matter content contains 150 g of solids and 0.85 L of water. If all the dry matter content was soluble sugar, the TSS of extracted juice would be 17.6 %w/v. In practice, mango fruit with 15 % w/w dry matter has a TSS of approximately 14 in juice of ripened fruit (Subedi et al., 2007), inferring around 3% w/w dry matter is associated with non-carbohydrate material, such as cell walls.

NIRS PLS models for dry matter content have been developed that are relatively robust to stage of ripening, i.e., to proportion of starch and soluble sugars. However, the accuracy of TSS models is decreased by variation in starch levels (e.g., in ripening apple and mango fruit, McGlone et al., 2002; Subedi and Walsh, 2011, respectively). This issue is presumably due to the similarity of NIRS spectra of starch and sugar in water. Thus, for fruit containing starch, accuracy and precision of NIR-TSS estimates is highest in fully ripe fruit, when all starch is converted to sugar (e.g., Subedi and Walsh, 2011). This 'interference' is not an issue in fruit that store soluble sugars rather than starch as their primary reserve, e.g., stonefruit or grape.

Internal defects: After dry matter and TSS levels, the Vis-NIRS based discriminant sorting of fruit on internal defects is the application that

Table 7
Parameters to be reported in a chemometric report on use of Vis-NIRS in a postharvest application, from the guidelines of Dardenne (2011) and Williams et al. (2017). The example of the attribute dry matter content is used.

Attribute, units	The attribute and its units. Units apply to RMSE and bias.
N	The number of samples (as reference analyses, not number of spectra). There may be more than one sample taken per fruit (e.g., two sides of a fruit). Replicate spectra of a sample should be averaged or contained within the same data set, i.e., not split between cross validation sets).
Range, average, SD	The minimum, maximum, average and SD of reference values for calibration and test populations.
Standard error of laboratory, SEL	The root mean square error (rmse) of replicate measurements of samples using the reference method.
Model type, #LVs or tuned parameters	The type of model used (e.g. NIPALS-PLSR or stepwise MLR) and parameter settings, e.g., number of latent variables used (with justification) for a PLSR model.
Wavelength range and step (nm)	The wavelength range or ranges chosen, with justification.
Outliers	The number of samples removed from a calibration set. Outliers can be removed on basis of an X residual (i.e., a spectral difference) as same rule can be applied in prediction. A justification should be provided for removal of outliers based on Y residual – this will reflect whether the goal of the model is to predict the average sample or the extreme samples well.
Pre-treatments	The pre-treatments employed should be listed, in the order employed, with some justification for their choice.
# CV folds	In LOO, the number of folds is N. RMSECV will increase with a decrease in the number of folds. In extreme, the folds can be independent groups, e.g., samples of different harvest events, in which case the outcome is equivalent to an averaged RMSEP.
Calibration and cross validation statistics	Calibration results (R^2_c, RMSEC) are often not reported in favour of CV results, but mention should be made of the difference between RMSEP or RMSECV and RMSEC. Cross validation results should include R^2_{cv} and RMSECV, and the ratio of SD to RMSECV.
Test set statistics	R^2_p, RMSEP, $RMSEP_{bc}$, bias, slope [$Y_{ref} = a + b.Y_{NIR}$] and the ratio of SD to RMSEP or $RMSEP_{bc}$. RSD, the residual standard deviation after slope and bias correction, may be reported. A Mahalanobois distance based measure of the test set is recommended, to indicate similarity of the test set to the calibration set.
NIR repeatability	The standard error of NIR estimated attribute level from repeated spectra acquisition of a sample. As a guideline, SE_{NIR} should be < 0.5 RMSECV.

has seen greatest commercial adoption, on packlines.

Both scattering and absorption influence the apparent absorption spectrum of a fruit. Internal features of the fruit that result in changes in light scattering within the fruit can be as detectable using Vis-NIRS as features related to absorbance. The internal defect of water core is associated with a decrease in the level of light scattering in a fruit and detection of this disorder by Vis-NIRS has been reported by a number of authors (e.g., Guo et al., 2020). Detection of other internal defects have also been reported, e.g., apple mouldy core (Shenderey et al., 2010) and apple internal browning (Khatiwadi et al., 2016).

Acidity: Acidity is a macro-constituent in fruit such as lemons and limes, which contain around 70 g L^{-1} (citric acid equivalents), but a micro-constituent in most fruit, e.g., the peach fruit assessed by Subedi et al. (2012b) had a mean acidity of 8.8 g L^{-1} (citric acid equivalents). A refractometer based TSS reading of lime juice is thus dominated by the contribution of organic acids and not soluble sugars, while the reverse is true for peach. The RMSEP of SWNIRS assessment of an independent population of intact and cut lime fruit was reported by Subedi et al. (2012a, 2012b) at 3.0 and 1.6 g L^{-1} (citric acid equivalents), respectively. Given this RMSEP value, the reliable direct assessment of acidity in fruit with lower levels of acidity is unlikely, where reliable refers to assessment of test sets not included in the calibration set. However, indirect assessment of acidity may have practical value, if the indirect association holds in practical use. An indirect assessment involves correlation of acidity level to another attribute that is assessable by Vis-NIRS, such as chlorophyll level.

Firmness: The non-invasive assessment of fruit firmness remains a 'holy grail' in postharvest research. The traditional method of assessment is destructive, involving insertion of a penetrometer into the fruit. There have been many claims for the assessment of fruit firmness using Vis-NIRS. Indeed, 10 % of all papers published in the period 2015–2020 involved assessment of firmness (Table 6).

Change in firmness is associated with minor changes in chemical composition, such as pectin levels. It is unlikely that NIRS can be used to detect these chemical changes in intact fruit. Change in firmness is also associated with change in cell wall adherence. Changes in cell shape might result in changes in the scattering of light within the fruit that could be detectable in the apparent absorbance spectrum, however such changes in scattering have not been consistently liked with firmness level. Firmness levels are correlated to a range of other attributes, from water content to pigment level and starch-sugar conversion during ripening, providing fertile ground for secondary Vis-NIRS correlations (e.g., Subedi and Walsh, 2008).

Thus, there is no consensus that firmness can be robustly (and directly) assessed using Vis-NIRS.

Other 'macro' attributes: Reasonable evidence is available in the literature that physiological states such as maturity or ripening stage and level of internal defects such as internal browning or water core can be assessed, with appropriate hardware, e.g., optical geometry.

Minor constituents: The direct assessment of minor constituents in intact, high moisture content fruit using Vis-NIRS is also unlikely, unless through indirect correlation to the level of another macro-constituent or pigment. For example, Ignat et al. (2012) reported an RMSECV of 15.1–18.9 mg per 100 g (fresh weight) for estimation of ascorbic acid in intact bell peppers using Vis-NIRS. The assessed fruit varied in maturity level. As many attributes vary during fruit maturation, the ascorbic acid assessment may effectively be of another attribute with correlation to ascorbic acid level. Lower detection limits should be possible in dry fruits.

The assessment of some minor constituents has been achieved using sample concentration techniques. For example, a NIRS assessment of surface fungicides on mango fruit was achieved of a dry extract of a solvent wash of fruit (Acharya et al., 2012).

Discrimination: There is often no need for a quantitative assessment of the level of an attribute, but rather a discriminant analysis is required for fruit sorting. The statistics of discriminant sorting is discussed by Walsh et al. (2020). There are increasing claims for discrimination of populations, e.g., on variety or species, geographic origin or production system, e.g., organic. However, robustness remains to be demonstrated in terms of successful application of such models on independent test sets. For example, the extent of internal browning in apple can be assessed by Vis-NIRS as either acceptable or not (Khatiwadi et al., 2016).

Future fruit properties: NIRS may be used to directly predict an attribute without direct *a priori* knowledge of the NIR assessed component. For example, Jacobs et al. (2016) reported on use of NIR spectra to predict storage life of lettuce. Such models need to be interpreted in terms of the underlying principle and demonstrated to be robust across populations to support practical adoption.

Combined attributes: Sometimes indices combining different quality parameters are useful. Vis-NIRS based models can be developed against the index itself, rather than the component attributes. For example, Cortés et al. (2016) developed Vis-NIRS based models on the IQI (internal quality index; Eq. 4) and the RPI (ripening index; eqn. 5), which are based on the attributes of penetrometer firmness (F), CIELAB color space L^* value, titratable acidity (TA), total soluble solids (TSS), and CIELCh colour space values $h_{ab}{}^*$ and $C_{ab}{}^*$.

$$\mathrm{IQI} = \ln\left(100 \cdot \mathrm{F} \cdot L^* \cdot h_{ab}{}^* \cdot \mathrm{TSS}^{-1} \cdot {C_{ab}}^{*-1}\right) \quad (4)$$

$$\mathrm{RPI} = \ln\left(100 \cdot \mathrm{F} \cdot \mathrm{TA} \cdot \mathrm{TSS}^{-1}\right) \quad (5)$$

5.7. NIRS special issue – water, H bonding and temperature

Water is the dominant NIR active molecule in fruit. Fleshy fruit contain around 80–90 % by weight water, and thus the measure of any other variable in fresh fruit is made against the large absorption features of water. Indeed, the increase of any fruit macro-constituent is associated with a decrease in the water content of the sample and the NIR assessment of a macro-constituents such as TSS and dry matter content may in practice rely strongly on a negative correlation with water.

The water absorption features are temperature sensitive. Water exists in several states associated with the degree of H bonding. The effect of increasing temperature (energy status) or soluble sugar concentration is a decreased level of H-bonding and a shift in the apparent O—H associated absorption peaks to shorter wavelengths (Golic et al., 2003). In practice, the impact of fruit temperature variation on a fruit dry matter prediction is primarily on accuracy (i.e., bias) rather than precision (i.e., bias corrected RMSEP) (e.g., Acharya et al., 2014a).

There are several approaches to deal with variation in sample temperature. The simplest approach is to include samples scanned at several temperatures into a 'global' model (Kawano, 2016), at a ratio of at least 500:1 (single temperature samples: multiple temperature samples) (Acharya et al., 2014a,b; Sun et al., 2020a, 2020b). Another approach requires development of a NIRS model on fruit temperature and estimation of predicted attribute bias per unit sample temperature change. NIR predicted fruit temperature can then be used in a calculation to adjust the predicted attribute level. Alternatively, various chemometric methods can be employed to remove the influence of temperature from spectra. Acharya et al. (2014a,Acharya et al., 2014b recommended use of a repeatability file over orthogonal scatter correction, generalized least square weighting and external parameter orthogonalisation, but the simple approach of a global model also produced good results.

5.8. NIR wavelength region

The SWNIR region (750 − 1100 nm) is used in commercial practice (see Section 3) for assessment of internal attributes of intact fruit such as TSS and dry matter content, in preference to the use of wavelengths > 1100 nm. However, most (57 %, Table 6) published reports on assessment of internal attributes of fruit involve instrumentation

employing longer (> 1000 nm) wavelength ranges. Longer wavelength ranges offer narrower and stronger absorption features than those observed in the SWNIR, and so may support superior performance in the assessment of internal quality attributes than use of the SWNIR. However, the absorption coefficient of water is relatively low in the SWNIR region, giving greater effective penetration depth into fruit. The lower effective penetration depth associated with use of longer wavelengths should limit performance robustness across independent populations, given variation in outer layer attributes. Even if similar results were obtained using the extended NIR region, the Vis-NIR option would be preferred for commercial purposes due to (currently) lower hardware cost (as noted by Ignat et al., 2014).

To clarify the issue of the optimal wavelength region for assessment of fruit internal quality attributes such as TSS and DM in the scientific literature, clear comparative studies are required. For example, better results were obtained using Vis-SWNIR than short wave IR reflectance spectroscopy for a bell-pepper application (Ignat et al., 2012). Better results were also reported using Vis-SWNIR than NIR for a carrot TSS application (Rady et al., 2018), for a grape color, phenolics, TSS and stage of ripeness application (Xiao et al., 2018) and for a persimmon astringency application (Cortés et al., 2017d). Better results were also obtained using the Vis-NIR than the NIR range for assessment of TSS of intact beets, while for cut slices of sugar beets, practically identical results were obtained (Pan et al., 2015), consistent with the effective penetration depth for these wavelength ranges. Conversely, Ignat et al. (2014) recorded a better result in assessment of apple parameters for a detector operating over the region 850 − 1888 nm than for a 340 − 1014 nm detector (using a reflectance geometry).

The comparison of wavelength ranges for an application usually involves use of different detectors and may involve use of different instruments. A comparison of results for different wavelength ranges must therefore separate the impact of different wavelength range from the impact of variation in other characters (e.g., repeatability, optical geometry and resolution). Settings should also be optimised separately for each wavelength range to achieve the same signal (and signal to noise) level, e.g., in a transmission geometry integration time should be set higher to optimise performance in longer wavelength regions, to the extent that the detector may be saturated with light at lower wavelengths.

5.9. Chemometrics

Typical data processing: The development of models relating spectra to attributes of interest is covered in the companion review of Saeys et al. (2020). In brief summary, the partial least squares regression (PLSR) technique is the dominant chemometric technique used in relating fruit spectra to attribute levels, with employ of a range of standard pre-processing techniques, typically mean centering, standard normal variate or multiplicative scattering correction and derivatives. Wavelength selection methods involving down sampling of spectral data to remove redundant data is also required for the optimisation of a given application, with a range of methods reported, e.g., Bexiga et al. (2017).

The optimization of pre-processing technique using standard approaches is not novel, and thus not the focus for a scientific research report, but it is a pre-requisite for NIRS application, and thus it should be briefly reported in application development reports. If a novel method is proposed, benchmarking to a standard method well represented in the literature is recommended. A useful illustration of such benchmarking is provided for an avocado application by Sun et al. (2020a). Whether a pre-processing procedure optimised for a PLSR model is also optimal for another model type (e.g., ANN) is an open question.

Modelling: PLSR is the most common chemometric modelling method employed in postharvest research studies (Table 6). Current commercial postharvest Vis-SWNIRS instrumentation exclusively employ PLSR or MLR techniques. In other food applications neural networks have been commercially deployed (e.g., Anderson, 2007), suggesting there is scope for further work with other multivariate techniques in postharvest applications, with benchmarking to PLSR using the same data set for calibration and independent test sets. Reports of applications of these modelling techniques in postharvest applications exist (e.g., Mukarev and Walsh, 2012), but consistent benefit over use of PLSR has not been demonstrated.

Other applications require classification rather than quantification of attribute level. The techniques of principal component regression (PCA), linear discriminant analysis (LDA), and PLS-DA are typically employed for such applications. For example, Cortés et al. (2017b,Cortés et al., 2017c differentiate cultivars of nectarine, while Timkhum and Terdwongworakul. (2012) classified durian fruit to maturity classes and Khatiwada et al. (2016) differentiated apple with internal browning.

Calibration transfer: Calibration transfer between instruments is a relatively under reported topic for postharvest applications. A difficulty for this application is that fresh fruit samples are unstable and can not be maintained as check samples as practiced with low moisture samples. Current recommendation is either a model updating procedure (existing model based on spectra from a master instrument updated using data from the slave unit) and/or appropriate wavelength selection based on orthogonal signal correction or a partial direct standardisation procedure involving use of a set of 'transfer' spectra scanned on both instruments to create a transfer function (e.g., Igne et al., 2009; Roger, 2016; Hayes et al., 2016). Further activity in this area is therefore warranted, both in terms of transfer between instruments of the same make/model and between different instruments.

Benchmarking: Comparison of the performance of methods or instruments reported in different publications is difficult given differences in the data sets of these reports (e.g., population structure). The machine vision community addresses this issue through a number of challenges involving access to open data sets (e.g., ImageNet Large Scale Visual Recognition Challenge, ILSVRC; http://image-net.org/challenges/LSVRC/) and similar open Vis-NIRS data sets, admittedly of a smaller scale, exist for other applications, e.g., for a soil application, Pierna and Dardenne (2008). To the authors knowledge, similar open data sets do not exist for postharvest examples. However, journals are encouraging submission of data sets associated to articles (e.g., https://data.mendeley.com/research-data/?search = fruit%20nirs), creating a resource for comparative chemometric studies.

Reporting requirements: The comparison of reports on the use of Vis-NIR spectroscopy requires use of a common language. Dardenne (2010) and Williams et al. (2017) provide useful guides to the requirements for reporting of a chemometric study, relevant for any postharvest report involving spectroscopy. Williams et al. (2017) note nearly 40 items that should be reported in a spectroscopic study to enable duplication of the application and for extension of the work to industrial application. These items range from characterization of the calibration and validation sets and characterisation of the model, e.g., number of terms used in, and b coefficients of a PLSR model, to reporting of performance statistics. These guides also comment on the need for consistency in use of chemometric terms and abbreviations. For example, labelling should distinguish between calibration, cross validation and independent test set results, e.g., for the coefficient of determination associated with a calibration, R^2_c; for cross validation, R^2_{cv} and for an independent test (or 'prediction') set result R^2_v or R^2_p.

Population standard deviation (SD) is integral to determining the value of the NIRS technique for sorting of fruit. The technique hold value only when sample variation (standard deviation, SD) in the attribute of interest is greater than the measurement RMSEP. Indeed, the R^2 of the prediction is directly related to measurement bias corrected RMSEP ($RMSEP_{bc}$) and SD (eqn. 3).

$$R^2 = 1 - (RMSEP_{bc}/SD)^2 \quad (3)$$

For example, if $RMSEP_{bc}$ = 1, and SD = 2, R^2 will be 0.75. For the same $RMSEP_{bc}$, and SD = 3, R^2 will be 0.89. Thus, if RMSEP = 1, the technique has no value for sorting of a population of SD = 1.0, but it has great value to sorting of a population of SD = 10. In consequence, the interpretation of calibration and validation statistics requires knowledge of population SD.

Calibration set size: Some reports of NIRS application development are based on a small number of samples in the calibration set. Consider that there is a reasonable chance that two random numbers will fall in ascending order. For an extreme case, consider if spectra of hundreds of wavelength data points were acquired of only three fruit spectra. There is a probability that values at some wavelengths will randomly trend with attribute level for those fruit. This represents over-fitting of multivariate regression models.

For assessment of intact fruit, it is recommended that application studies include in the order of hundreds of spectra paired to reference values. Practical use of a model will require inclusion of data from multiple harvests or seasons to produce a 'robust' model, resulting in data sets of many hundreds of samples (e.g., Peirs et al., 2003; Subedi et al., 2007; Blakey, 2016). Thus, a comparison of PLS, MLR and LS-SVM modelling approaches based on spectra of 120 fruit collected at one location and time, with division to calibration and validation sets based on a ranking of reference (TSS) values (Hu et al., 2019) will provide prediction results that are optimistic relative to use in prediction of independent sets, and it is unclear if the proposed solution will hold in practical use. Blakey (2016) provides a useful case study employing nearly 10,000 samples with use of independent test sets for an avocado dry matter content application. Cross validation routines help avoid this issue, but the cross-validation groups should be large, ideally based on distinct groups of data, rather than, for example, single sample cross validation.

An indication of insufficient numbers in the calibration set is provided by a RMSEP or RMSECV value that is substantially higher than the RMSEC value is. Papers rarely present both RMSEC and RMSECV but at a comment on the difference between the values should be made in justification of the sample size used.

Independent test sets: For practical implementation, a Vis-NIRS model should be 'robust' in use across production conditions, seasons, storage conditions, plant varieties and instruments, as well as measurement conditions such as ambient light and temperature. Demonstration of model robustness is a prerequisite to adoption of the technology by the postharvest industry and should be a focus of current and future studies. Many reviews have stressed the need for an independent test set, unused in tuning of model parameters, to generate prediction statistics (e.g., Williams et al., 2017).

The majority of publications (66 %; with 68 % of those reports using leave one out (LOO) cross validation) are based on cross validation results only, and most remaining publications (22 % of total) deliberately select their test sets to be representative of the calibration set (e.g., ranking of samples by attribute level followed by selection of every third sample for the test set). For example, Clark et al. (2003) utilized fruit of four harvests (n = 180), with random splits of each harvest set to create the calibration (n = 120) and validation (n = 60) sets (Table 6). Validation using within-population sets will provide an indication of model performance that is optimistic in comparison to use with independent tests sets, as must happen in practical implementation.

The selection of test sets that mirror the intended use of the model is therefore recommended, e.g., in a NIRS pack-line implementation, a model will be used in prediction of fruit from different harvest dates, growing locations and conditions and perhaps of different cultivars. Such fruit may vary in chemical matrix or in light scattering properties, e.g., change in the soluble sugar types or the level of organic acids can impact a refractometric assessment of TSS, or skin properties may change with water stress, changing scattering coefficients.

Several reports indicate that inclusion of three years (growing seasons) of data is required to create a robust model on standard parameters such as TSS and DM (e.g., Peirs et al., 2003; Subedi et al., 2007), although this result may also be linked to the duration of a standard funding grant. Some attempts have been made to create robustness within a single season by including samples from range of water stress treatments (Anderson et al., 2017) and maturation/ripeness stages in the calibration set.

It is recommended that future application development studies include multiple populations. Results should be reported in terms of prediction statistics for these sets, or as cross validation results using the independent sets as cross validation groups. The results for the separate tests sets should be used to tease out the conditions that cause NIRS model accuracy or precision to decrease (e.g., sensitivity to variety, growing location, season, instrument ageing).

6. Conclusions and recommendations

6.1. Expected future advances

Instrumentation for colour measurement and Vis-NIRS spectroscopy has become widely available, and at decreasing cost. This availability has supported an increase postharvest research literature. These measurement technologies were initially commercially applied in the packhouse, but with the advent of handheld technology, adoption is now occurring throughout the postharvest value chain, both upstream to the orchard and downstream to distribution centers and to consumer use. Future advances in technology promise further miniaturization, enabling integration of spectrometers into other devices.

Multiple cameras and sensors are used in fruit pack-lines, and the trend to use of multiple probes in assessment of fruit is likely to continue, extending from packhouse to other points in the value chain. For example, Cortés et al. (2017a) integrated two Vis-NIR spectrometric probes to view opposite sides of a mango fruit in a robotic harvesting arm. An accelerometer was incorporated to assess fruit firmness and data combined into a measure of the overall quality of the fruit. The system was impractical (9 s per evaluation) but is indicative of the potential for multiple measurements and sensor fusion.

Advances in wireless connectivity is allowing the use of cloud computing for model predictions, either in context of enabling a simpler spectrometer, as seen in the SCiO unit (Table 4), or in context of device agnostic services that offer more complex chemometric modelling techniques, e.g., Hone (https://www.honeag.com/hone-create/; doa 19/03/20).

6.2. Recommendations for future application development work

The following areas are recommended in future documentation on development of Vis-NIR region 'point' spectroscopy applications:

Procedure

(i) The error associated with the reference method (SEL) should be documented.
(ii) Inter-correlations of the attribute of interest with other Vis-NIR active attributes should be documented, e.g., with pigment level or water content. Assessment of an attribute of interest with a strong secondary correlation to a Vis-NIRS assessable attribute will be robust only if the attribute of interest is always correlated to the attribute of interest.
(iii) Spatial variation within the product (i.e., within a single fruit) of the attribute of interest should be described, with consideration of factors such as product maturity and storage time, and the sampling position on the fruit for point spectroscopy should be justified in terms of representation of the whole fruit.
(iv) The physically sampled tissue volume used for the reference method should be matched to the optically sampled volume.

Equipment

(v) In some published studies, it appears that the spectrometer was selected because it was available, not because the instrument was matched to the application. The choice of spectrometer should be justified, and specifications of the spectrometer used should be documented in terms of repeatability (e.g., SD of Absorbance of 20 repeated measurements of a white reference, optical resolution as FWHM and pixel resolution), to enable a level of comparison with other published studies.

(vi) The following instrumentation characteristics are offered as a benchmark condition, to be challenged for a particular fruit application:
- a full or partial transmission optical geometry over a reflection geometry
- use of the SWNIR region for improved depth of penetration into the sample and lower cost hardware
- an optical resolution at least 10 nm and a repeatability (SD of repeated reference spectra) of at least 10 mAbs (Greensill and Walsh, 2000)
- use of instruments with higher wavelength resolution to improve calibration transfer between instruments.

Most current studies on use of Vis-NIRS to assess intact fruit (see Section 3) utilize a reflection geometry and a long wavelength region (1100–2500 nm). This is likely to result in spectra dominated by absorption features of the fruit skin, and thus less robust models if skin properties change between populations. Nonetheless, the 'proof is in the pudding', and any geometry or instrumental wavelength range that results in a good prediction result of populations independent of the calibration set is acceptable. Further work involving direct comparisons of geometries and other instrumentation characters is warranted to achieve consensus in these areas.

Statistical reporting

(vii) Dardenne (2011) and Williams et al. (2017) have stressed the need for consistency in use of chemometric terms and abbreviations. Table 7 provides a summary of these two guides in context of a postharvest applications.

(viii) At the very least, prediction results should be reported in terms of population mean and SD, with prediction statistics of R_p^2, RMSEP and bias.

(ix) The wavelength range selected and pre-treatments used (e.g., use of % transmission compared to absorbance, SNV, MSC, level of derivative) should be optimized, with reporting avoiding the detail of these comparisons, but including what was considered and the best result.

(x) Terminology should be used to avoid confusion between reference method and NIRS based estimates of an attribute, e.g., refractometer–TSS and NIR–TSS, or oven–DM and NIR–DM.

Validation and transfer

(xi) The adage of 'no interpretation without prediction and no prediction without interpretation' should be followed. Models should be tested on independent sets of fruit, i.e., different harvest events or storage conditions, and not only on sets drawn from the populations used in calibration. Interpretation involves an understanding of the principle behind the model, with interpretation of in context of spectroscopic features and model coefficients.

(xii) Models should be tested in a range of usage conditions (e.g., fruit and instrument temperatures, ambient light levels, different models of the same instrument, fruit pose), i.e., reports should involve multiple validation populations.

(xiii) Calibration model transfer between instruments should be demonstrated and optimized.

Declaration of Competing Interest

Co-author Walsh acknowledges involvement in the development of the F750 instrument with Felix Instruments and involvement with MAF RODA. We believe this potential bias is balanced by the input of the two other authors.

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